9-tert-Butyl-1-oxaspiro[4.5]deca-6,9-dien-2,8-dion

Inchi: InChI=1S/C13H16O3/c1-12(2,3)9-8-13(6-4-10(9)14)7-5-11(15)16-13/h4,6,8H,5,7H2,1-3H
InchiKey: IUQXVAIQPMFIGU-UHFFFAOYSA-N
Formula: C13H16O3
SMILES: CC(C)(C)C1=CC2(C=CC1=O)CCC(=O)O2
Mol. weight [g/mol]: 220.26

Physical Properties

Property code	Value	Unit	Source
gf	-144.27	kJ/mol	Joback Method
hf	-467.17	kJ/mol	Joback Method
hfus	11.57	kJ/mol	Joback Method
hvap	57.16	kJ/mol	Joback Method
log10ws	-2.77		Crippen Method
logp	2.174		Crippen Method
mcvol	172.720	ml/mol	McGowan Method
pc	2796.51	kPa	Joback Method
rinpol	1932.00		NIST Webbook
rinpol	1929.00		NIST Webbook
tb	694.97	K	Joback Method
tc	959.23	K	Joback Method
tf	465.68	K	Joback Method
vc	0.640	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	498.23	J/mol×K	694.97	Joback Method
cpg	516.85	J/mol×K	739.01	Joback Method
cpg	534.36	J/mol×K	783.06	Joback Method
cpg	550.96	J/mol×K	827.10	Joback Method
cpg	566.83	J/mol×K	871.14	Joback Method
cpg	582.16	J/mol×K	915.18	Joback Method
cpg	597.15	J/mol×K	959.23	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R576711&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume